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EVANSTON IL DEPT OF ENGINEERING SCIENCE AND..
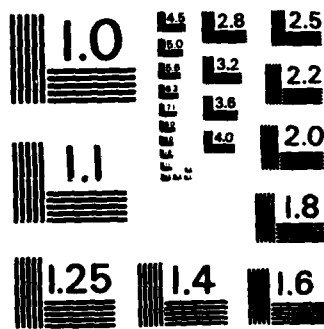UNCLASSIFIED B J MATKOWSKY APR 85 AFOSR-TR-85-0767 F/G 12/1 NL

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FIELD	GROUP	SUB. GR.	random phenomena, asymptotic methods, atomic migration chemical reaction rates

19. ABSTRACT (Continue on reverse if necessary and identify by block number)

The goal of our study was to develop new asymptotic and singular perturbation methods for the analysis of random phenomena, and their application in various areas of science and engineering. We have studied the problems of (1) atomic migration in crystals, (2) ionic and super-ionic conductivity, (3) chemical reaction rates, surface desorption rates, and more general activated rate processes, (4) noise effects on the hysteretic Josephson junction, D.C.-SQUID, and other tunnel junction devices, (5) stability and reliability of randomly loaded elastic structures, (6) relative stability of various multi-stable systems, among others. Considerable success has been achieved, not only in developing new mathematical methods, but in solving a number of problems whose solution has been long outstanding. These include the Kolmogorov Exit Problem and the Kramers nonlinear diffusion problem, among others.

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FINAL REPORT

AIR FORCE OFFICE OF SCIENTIFIC RESEARCH

AFOSR 83-0086

"FIRST PASSAGE TIMES IN STOCHASTIC DIFFERENTIAL EQUATIONS

OF MATHEMATICAL PHYSICS AND ENGINEERING"

Principal Investigator

Bernard J. Matkowsky
Department of Engineering Sciences and Applied Mathematics
The Technological Institute
Northwestern University
Evanston, IL 60201

April 1985

Final Report

Air Force Office of Scientific Research Grant AFOSR 83-0086, entitled
"First Passage Times in Stochastic Differential Equations of Mathematical
Physics and Engineering"

Principal Investigator: Prof. Bernard J. Matkowsky
                           Dept. of Engineering Sciences and Applied
                             Mathematics
                           The Technological Institute
                           Northwestern University
                           Evanston, IL 60201

   Under this grant, we supported the successful collaboration between
Professors B. J. Matkowsky and Z. Schuss on Singular Perturbation Methods in
Stochastic Differential Equations and Applications to various scientific
disciplines. We made a number of breakthroughs on some fundamental problems,
both in science and in mathematics.

   The goal of our study was to develop new asymptotic and singular
perturbation methods for the analysis of random phenomena, and their appli-
cation in various areas of science and engineering. We have studied the
problems of (1) atomic migration in crystals, (2) ionic and super-ionic
conductivity, (3) chemical reaction rates, surface desorption rates, and
more general activated rate processes, (4) noise effects on the hysteretic
Josephson junction, D.C.-SQUID, and other tunnel junction devices, (5) stability
and reliability of randomly loaded elastic structures, (6) relative stability
of various multi-stable systems, among others. Considerable success has been
achieved, not only in developing new mathematical methods, but in solving a
number of problems whose solution has been long outstanding. These include
the Kolmogorov Exit Problem and the Kramers nonlinear diffusion problem,
among others. The problems above, are modelled by stochastic differential
equations, describing continuous dynamical systems.

   We also developed new methods for the study of stochastic difference
and integro-differential-difference equations describing discrete systems,
modelled by master equations. We studied new applications of these methods
to (A) large communication and computer networks, and their scheduling, and
(B) problems of large deviations in statistical testing, estimation and
sequential sampling. In addition, master equations serve as a more funda-
mental description of the physical and chemical processes described above.
In certain instances, the continuous description can be shown to be a limiting
approximation of the discrete system, the so-called diffusion approximation.
In other instances, however, this approximation procedure, though widely used,
can be shown to yield results which are incorrect by orders of magnitude.
We have given conditions for the validity, as well as the limitations, of
this approximation, and when the approximation is not valid, we have provided
new procedures for dealing directly with the underlying stochastic difference
equations. A list of publications and abstracts now follows.

1. "Uniform expansion of the transition rate in Kramers problem," J. Statis. Physics 35, (1984) pp. 443-456.

    Kramers' model of diffusion over potential barriers, e.g. chemical reactions, based on the noise activated escape of a particle from a potential well, is considered. Kramers derived escape rates valid for intermediate and large damping, and in a separate analysis, for small damping. In the small damping limit, Kramers' intermediate result reduces to the transition-state rate which does not agree with the small damping result. A new escape rate is derived that is uniformly valid for all values of the damping coefficient. The new rate reduces to Kramers' results in the appropriate limits and, in particular, connects Kramers' intermediate and small damping results.

2. "Solution of Kramers Moyal equations for problems in chemical physics," J. Chemical Physics 81 (1984) pp. 1285-1293.

    We derive asymptotic solutions of Kramers-Moyal equations (KMEs) that arise from master equations (MEs) for stochastic processes. We consider both one step processes, in which the system jumps from x to $x + \epsilon$ or $x-\epsilon$ with given probabilities, and general transitions, in which the system moves from x to $x + \epsilon\xi$, where ξ is a random variable with a given probability distribution. Our method exploits the smallness of a parameter ϵ, typically the ratio of the jump size to the system size. We employ the full KME to derive asymptotic expansions for the stationary density of fluctuations about, as well as for the mean lifetime of stable equilibria. Thus we treat fluctuations of arbitrary size, including large fluctuations. In addition we present a criterion for the validity of diffusion approximations to master equations. We show that diffusion theory can not always be used to study large deviations. When diffusion theory is valid our results reduce to those of diffusion theory. Examples from macroscopic chemical kinetics and the calculation of chemical reaction rates ("Kramers" models) are discussed.

3. "Asymptotic analysis of the optimal filtering problem for one-dimensional diffusions measured in a low noise channel, Part II", SIAM J. Appl. Math. 44, (1984) pp. 1176

    We consider the problem of filtering one-dimensional diffusions with nonlinear drift coefficients, transmitted through a nonlinear low noise channel. We construct an asymptotic solution to Zakai's equation for the unnormalized conditional probability density of the signal, given the noisy measurements. This expansion is used to find the asymptotic expansion of the minimum error variance filter and its mean square estimation error (MSEE). We construct approximate filters whose MSEE agrees with that of the optimal one to a given degree of accuracy. The dimension of the approximate filter increases with the required degree of accuracy. Similarly, we expand the maximum a posteriori probability estimator and the minimum energy estimator and compare their performance. We also discuss some extended Kalman filters and present some examples.

4. "Asymptotic solution of the Kramers-Moyal equation and first passage
    times for Markov jump processes," Physical Rev. A 29 (1984), pp. 3359

    We calculate the activation rates of metastable states of general one-
    dimensional Markov jump processes by calculating mean first-passage times.
    We employ methods of singular perturbation theory to derive expressions
    for these rates, utilizing the full Kramers-Moyal expansions for the
    forward and backward operators in the master equation. We discuss various
    boundary conditions for the first-passage-time problem, and present some
    examples. We also discuss the validity of various diffusion approxi-
    mations to the master equation, and their limitations.

5. "First passage times for processes governed by Master Equations,"
    Springer Proceedings in Physics #1, (1984) pp. 19-36.

    We calculate the activation rates of metastable states of processes
    governed by Master Equations, by calculating mean first passage times.
    We employ methods of singular perturbation theory to derive expressions
    for these rates, utilizing the full Kramers-Moyal expansions for the
    forward and backward operators in the Master Equation. In addition
    we discuss the validity of various diffusion approximations to the
    Master Equation, showing that such approximations are not valid in
    general.

6. "Noise-induced transitions in multi-stable systems," Springer Proceedings
    in Physics #1 (1984) pp. 79-94.

    The damped physical pendulum driven by constant torque serves as a model
    for many physical systems (e.g., the motion of an ion in a crystal subject
    to a uniform electrostatic field, the point Josephson junction driven
    by constant current, charge density waves, etc.). For certain ranges
    of parameters it has both stable equilibrium states and a stable non-
    equilibrium state. In the presence of a random driving force of thermal
    or shot noise type there are transitions between the stable states of
    the pendulum. We calculate the steady state distribution of fluctuations
    about the stable staes and the transition rates between them. For
    the point Josephson junction at very low temperatures we postulate the
    existence of "self-generated" shot noise and obtain transition rates
    which agree with the experimental results of Voss and Webb. This
    paper summarizes the work of Ben-Jacob, Bergman, Imry, Knessl, Matkowsky
    and Schuss.

7. "Frequency fluctuations in noisy oscillators," SIAM J. Appl. Math.,
    to appear.

    We study frequency and period fluctuations in a nonlinear oscillator
    driven by Gaussian white noise. We define the random period as the
    random time between two consecutive zero crossing by the random
    phase plane trajectory, and the random frequency as the number of such
    zero crossings per unit of time. These quantities are shown to be
    related by renewal theory. We find asymptotic expressions for the means
    and variances of the random period and random frequency, for small damping
    and small noise. The formulas are particularly useful for oscillators
    with high frequency.

8. "An asymptotic theory of large deviations for Markov jump processes,"
SIAM J. Appl. Math., to appear.

We present new asymptotic methods for the analysis of Markov jump
processes. The methods, based on the WKB and other singular perturbation
techniques, are applied directly to the Kolmogorov equations and not
to approximate equations that come e.g. from diffusion approximations.
For time homogeneous processes, we construct approximations to the
stationary density function and the mean first passage time from a given
domain. Examples involving a random walk and a problem in queueing theory
are presented to illustrate our methods. For a class of time inhomogeneous
processes, we construct long time approximations to the transition
probability density function and the probability of large deviations
from a stable state. The law of large numbers is obtained as a special case.

9. "Asymptotic analysis of a state-dependent M/G/1 queueing system,"
submitted for publication.

We present new asymptotic methods for the analysis of queueing systems.
These methods are applied to a state-dependent M/G/1 queue. We formulate
problems for and compute approximations to (i) the stationary density
of the unfinished work; (ii) the mean length of time until the end of a
busy period; (iii) the mean length of a busy period; (iv) the mean time
until the unfinished work reaches or exceeds a specified capacity;
and (v) the distribution of the maximum. The methods are applied to
the full Kolmogorov equations, scaled so that the arrival rate is rapid
and the mean service is small. Thus, we do not truncate equations as in
diffusion approximations. We specialize the results to state-dependent
M/M/1 queues. For state-independent M/M/1 queues, we demonstrate theiry
accuracy by comparison with known exact solutions and results obtained
using diffusion approximations.

10. "System crash in a finite capacity M/G/1 queue," submitted for publication.

We analyze a finite capacity, M/G/1 queueing system in which an arrival
that causes the system capacity of unfinished work to be exceeded results
in the loss of all jobs circulating in the system, i.e., the system
"crashes". Problems are formulated for the stationary density of
unfinished work, the system utilization, the mean length of the busy
period, the mean total unfinished work in the system during a busy period,
and the probability that the system crashes before completing a busy
period. We construct exact solutions for these quantities for an M/M/1
queue with constant arrival and service rates. Approximate expressions
for these quantities are constructed for M/G/1 queues in which the
arrival rates and service densities depend on the amount of unfinished
work in the system at the instant a new customer enters the system.
These approximate expressions, which are obtained by using singular
perturbation techniques, are shown to agree with the exact results for
state-independent M/M/1 queues.

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